


MS/MS biclustering and molecular networking

DL Dapeng Li

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 An abbreviated version of this protocol was published in Science Advances in Jun 2020

Information theory tests critical predictions of plant defense theory for specialized metabolism

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Detailed protocol

Thank you for your interests in our "MS/MS biclustering and molecular networking" analysis in our article of "Information theory tests critical predictions of plant defense theory for specialized metabolism".

In this biclustering analysis, we used previously published open source R method termed DiffCoEx which builds on the commonly used Weighted Gene Coexpression Network Analysis (WGCNA) framework for coexpression analysis and considers coexpression differences in two conditions (here MS/MS fragment similarity and MS/MS neutral loss similarity, respectively). The original script of DiffCoEx can be downloaded from the additional file 1 in the DiffCoEx publication which includes Step-by-step R analysis for applying DiffCoEx (<https://bmcbioinformatics.biomedcentral.com/articles/10.1186/1471-2105-11-497>). The resulted biclustering matrix can be then used as input for the Molecular networking analysis which was conducted using Cytoscape software. It is also recommended to use the GNPS (<https://gnps.ucsd.edu/ProteoSAFe/static/gnps-splash.jsp>) website to conduct such a molecular networking analysis which is a web-based MS/MS ecosystem that integrates many MS/MS data analysis tools. In order to provide a more detailed and straightforward script for the exact MS/MS biclustering and molecular networking analysis in our analysis, we have uploaded an R script with detailed step by step annotation which was used to conduct such an analysis as shown in Fig.3E in our recent publication (<https://science.sciencemag.org/content/371/6526/255/tab-article-info>). The R script can be downloaded via this link as "Fig3E.R" (<https://doi.org/10.6084/m9.figshare.13414670.v1>).

We hope this detailed script with annotation would provide sufficient information to guide interested readers.

If there are further questions, please don't hesitate to reach out.

Contacting Dapeng Li at dli@ice.mpg.de from March 20-July 5th 2021, when Ian is running the field work in Utah, where the internet access is very poor, would probably be best.

How to cite: (Readers should cite both the Bio-protocol preprint and the original research article where this protocol was used)

1. Li, D. (2021). MS/MS biclustering and molecular networking. Bio-protocol Preprint. bio-protocol.org/prep937.
2. Li, D., Halitschke, R., Baldwin, I. T. and Gaquerel, E. (2020). Information theory tests critical predictions of plant defense theory for specialized metabolism. Science Advances 6(24). DOI: [10.1126/sciadv.aaz0381](https://doi.org/10.1126/sciadv.aaz0381)

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